

10/584440

=> file registry

FILE 'REGISTRY' ENTERED AT 10:45:40 ON 19 FEB 2008
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7
DICTIONARY FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file caplus

FILE 'CAPLUS' ENTERED AT 10:45:42 ON 19 FEB 2008
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FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L30

L21	4	SEA FILE=CAPLUS ABB=ON	PLU=ON	BLEGER F?/AU
L22	2	SEA FILE=CAPLUS ABB=ON	PLU=ON	MORDACQ F?/AU
L23	66	SEA FILE=CAPLUS ABB=ON	PLU=ON	PIRON J?/AU
L26	37	SEA FILE=CAPLUS ABB=ON	PLU=ON	SCHOUTEETEN A?/AU
L27	2	SEA FILE=CAPLUS ABB=ON	PLU=ON	L21 AND (L22 OR L23 OR L26)
L28	2	SEA FILE=CAPLUS ABB=ON	PLU=ON	L22 AND (L23 OR L26)

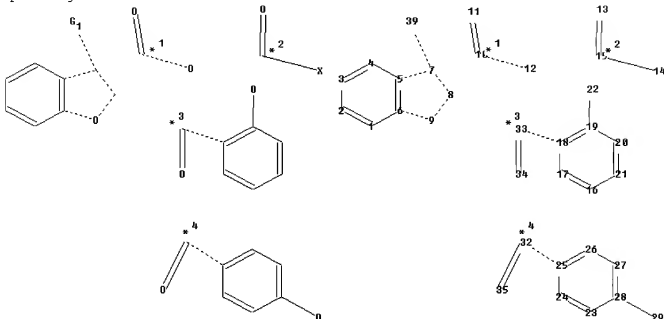
10/584440

L29 1 SEA FILE=CAPLUS ABB=ON PLU=ON L23 AND L26
 L30 3 SEA FILE=CAPLUS ABB=ON PLU=ON (L27 OR L28 OR L29)

=> d stat que L31
 L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
 Uploading L1.str



chain nodes :
 10 11 12 13 14 15 22 29 32 33 34 35 39
 ring nodes :
 1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 28
 chain bonds :
 7-39 10-12 10-11 13-15 14-15 18-33 19-22 25-32 28-29 32-35 33-34
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 16-17 16-21 17-18 18-19 19-20
 20-21 23-24 23-28 24-25 25-26 26-27 27-28
 exact/norm bonds :
 5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-35
 33-34
 exact bonds :
 14-15
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 23-24 23-28
 24-25 25-26 26-27 27-28

G1:[*1],[*2],[*3],[*4]

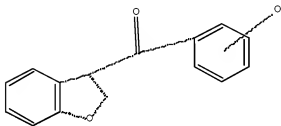
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
 19:Atom 20:Atom 21:Atom

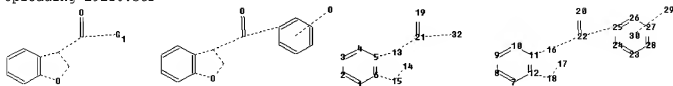
10/584440

22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS
 33:CLASS
 34:CLASS 35:CLASS 39:CLASS

L5 8858 SEA FILE=REGISTRY SSS FUL L1
 L9 STR



Structure attributes must be viewed using STN Express query preparation:
 Uploading L9L10.str



chain nodes :

19 20 21 22 29 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27
 28

chain bonds :

13-21 16-22 19-21 20-22 21-32 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-13 6-15 7-8 7-12 8-9 9-10 10-11 11-12 11-16
 12-18 13-14 14-15 16-17 17-18 23-24 23-28 24-25 25-26 26-27 27-28

exact/norm bonds :

5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-22
 21-32 22-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 23-24 23-28 24-
 25
 25-26 26-27 27-28

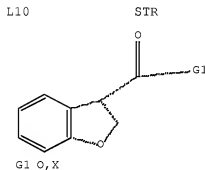
G1:O,X

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
 20:CLASS 21:CLASS
 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
 32:CLASS

10/584440

fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
node mappings:
14:17 13:16



Structure attributes must be viewed using STN Express query preparation.

L12	1802	SEA FILE=REGISTRY SUB=L5 SSS FUL L9
L14	7056	SEA FILE=REGISTRY SUB=L5 SSS FUL L10
L17	230	SEA FILE=CAPLUS ABB=ON PLU=ON L12 (L) PREP/RL
L18	312	SEA FILE=CAPLUS ABB=ON PLU=ON L14 (L) (RACT OR RGT OR RCT)/RL
L19	5	SEA FILE=CAPLUS ABB=ON PLU=ON L17 AND L18
L21	4	SEA FILE=CAPLUS ABB=ON PLU=ON BLEGER F?/AU
L22	2	SEA FILE=CAPLUS ABB=ON PLU=ON MORDACQ F?/AU
L23	66	SEA FILE=CAPLUS ABB=ON PLU=ON PIRON J?/AU
L26	37	SEA FILE=CAPLUS ABB=ON PLU=ON SCHOUTEETEN A?/AU
L31	1	SEA FILE=CAPLUS ABB=ON PLU=ON L19 AND (L21 OR L22 OR L23 OR L26)

=> s L30 or L31
L36 3 L30 OR L31

=> file casreact
FILE 'CASREACT' ENTERED AT 10:46:02 ON 19 FEB 2008
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FILE CONTENT:1840 - 16 Feb 2008 VOL 148 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

10/584440

```
*
*   CASREACT now has more than 13.8 million reactions   *
*
*****
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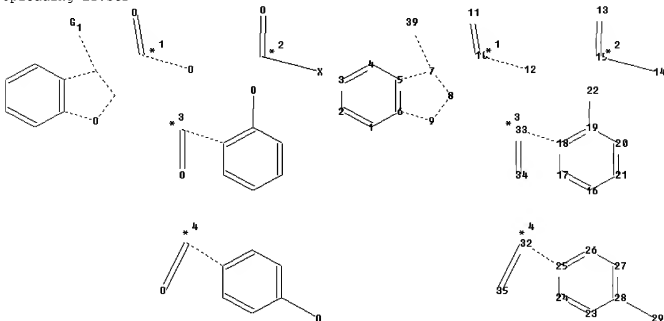
Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> d stat que L35
L1          STR
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



```
chain nodes :
10 11 12 13 14 15 22 29 32 33 34 35 39
ring nodes :
1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 28
chain bonds :
7-39 10-12 10-11 13-15 14-15 18-33 19-22 25-32 28-29 32-35 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 16-17 16-21 17-18 18-19 19-20
20-21 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-35
33-34
exact bonds :
14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 23-24 23-
28
24-25 25-26 26-27 27-28
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10/584440

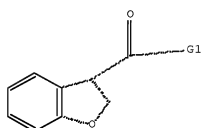
G1:[*1],[*2],[*3],[*4]

Match level :

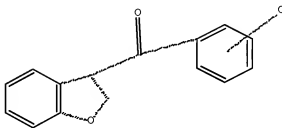
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 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
 19:Atom 20:Atom 21:Atom
 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS
 33:CLASS
 34:CLASS 35:CLASS 39:CLASS

L3

STR

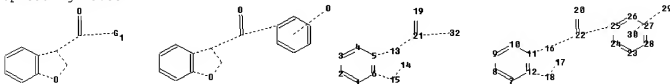


G1 O, X



Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



chain nodes :

19 20 21 22 29 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27 28

chain bonds :

13-21 16-22 19-21 20-22 21-32 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-13 6-15 7-8 7-12 8-9 9-10 10-11 11-12 11-16
 12-18 13-14 14-15 16-17 17-18 23-24 23-28 24-25 25-26 26-27 27-28

exact/norm bonds :

5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-22
 21-32 22-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 23-24 23-28 24-25
 25-26 26-27 27-28

10/584440

G1:O,X

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
32:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
node mappings:
14:17 13:16

L5 8858 SEA FILE=REGISTRY SSS FUL L1
L6 324 SEA FILE=CASREACT ABB=ON PLU=ON L5
L8 2 SEA FILE=CASREACT SUB=L6 SSS FUL L3 (8 REACTIONS)
L34 1 SEA FILE=CASREACT ABB=ON PLU=ON ("143:97254"/AN OR "2005:5690
50"/AN)
L35 1 SEA FILE=CASREACT ABB=ON PLU=ON L34 AND L8

=> d ibib abs hitstr L36 1-3; d ibib abs hit L35 1
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L36 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:569050 CAPLUS Full-text
DOCUMENT NUMBER: 143:97254
TITLE: Process for preparation de 2-(n-alkyl)-3-(4-
hydroxybenzoyl)benzofurans and intermediates by
halogenation of carboxybenzofuran derivatives,
Friedel-Crafts acylation with alkoxybenzenes and
dealkylation
INVENTOR(S): Schouteeten, Alain; Blegier, Francois; Mordacq,
Francoise; Pixon, Jerome
PATENT ASSIGNEE(S): Clariant France, Fr.
SOURCE: Fr. Demande, 22 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2864536	A1	20050701	FR 2003-15398	20031224
FR 2864536	B1	20060317		
WO 2005066149	A1	20050721	WO 2004-IB4158	20041215

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
 MR, NE, SN, TD, TG

EP 1699772 A1 20060913 EP 2004-801395 20041215
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS

CN 1898226 A 20070117 CN 2004-80038285 20041215
 JP 2007517012 T 20070628 JP 2006-546365 20041215
 NO 2006002936 A 20060922 NO 2006-2936 20060623
 IN 2006CN02324 A 20070706 IN 2006-CN2324 20060626
 US 2007155831 A1 20070705 US 2006-584440 20061129
 PRIORITY APPLN. INFO.: FR 2003-15398 A 20031224
 WO 2004-IB4158 W 20041215

OTHER SOURCE(S): CASREACT 143:97254
 GI

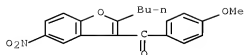
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is related to the preparation of benzofurans I [R = linear or branched alkyl; R1 = halo, NO2, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C6H5OR2 (III) [R2 = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R1, R2 defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO2; R4 = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5-nitrobenzofuran with SOCl2 in PhCl, acylation of anisole with acyl chloride in the presence of AlCl3, and demethylation over AlCl3 at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO2, R = n-Bu] after purification. Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)-benzofuran in the presence of acetic anhydride/H2SO4 for 2 h gave acid II (m.p. = 207°).

IT 141627-42-1P, 2-(n-Butyl)-3-(4-methoxybenzoyl)-5-nitrobenzofuran
 856758-82-6P, 2-(n-Butyl)-3-carboxy-5-nitrobenzofuran
 856758-83-7P, 2-(n-Butyl)-3-chlorocarbonyl-5-nitrobenzofuran
 856758-84-8P, 2-(n-Butyl)-3-(2-methoxybenzoyl)-5-nitrobenzofuran
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); FACT (Reactant or reagent)
 (intermediate; process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

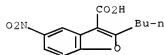
RN 141627-42-1 CAPLUS
 CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)

10/584440



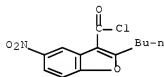
RN 856758-02-6 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-butyl-5-nitro- (CA INDEX NAME)



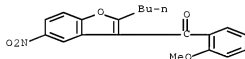
RN 856758-03-7 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-butyl-5-nitro- (CA INDEX NAME)



RN 856758-04-8 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(2-methoxyphenyl)- (CA INDEX NAME)



IT 956758-05-9F, 2-(n-Butyl)-3-(2-hydroxybenzoyl)-5-nitrobenzofuran

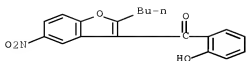
RL: BYP (Byproduct); IMF (Industrial manufacture); RCT (Reactant);

PPEP (Preparation); RACT (Reactant or reagent)

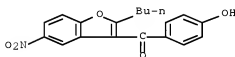
(process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

RN 856758-05-9 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(2-hydroxyphenyl)- (CA INDEX NAME)



IT 141645-16-1P, 2-(n-Butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (product; process for preparation de 2-(n-alkyl)-3-(4-
 hydroxybenzoyl)benzofurans and intermediates by halogenation of the
 corresponding carboxybenzofurans, Friedel-Crafts acylation with
 alkoxybenzenes and dealkylation)
 RN 141645-16-1 CAPLUS
 CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX
 NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:1018469 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 141:425581
 TITLE: Process for separating glyoxal diacetals from crude
 mixtures by countercurrent liquid-liquid extraction
 INVENTOR(S): Simon, Olivier; Bieger, Francois; Schouteeten, Alain
 PATENT ASSIGNEE(S): ClariantFrance, Fr.
 SOURCE: Fr. Demande, 22 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2855171	A1	20041126	FR 2003-6168	20030522
FR 2855171	B1	20050805		
WO 2004106274	A1	20041209	WO 2004-FR1224	20040518

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
 GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,

SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

EP 1625108 A1 20060215 EP 2004-742769 20040518
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

CN 1795157 A 20060628 CN 2004-80014034 20040518
 JP 2007502318 T 20070208 JP 2006-530363 20040518
 US 2007073088 A1 20070329 US 2005-557920 20051122
 IN 2005CN03483 A 20070914 IN 2005-CN3483 20051222

PRIORITY APPLN. INFO.: FR 2003-6168 A 20030522
 WO 2004-FR1224 W 20040518

AB (RO)2CHCH(OR)2 (R = C1-4 alkyl) is separated from acetalization product mixts. also containing (RO)2CHCHO (R = C1-4 alkyl) by discontinuous or continuous countercurrent liquid-liquid extraction using solvents not miscible with the reaction media.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:524688 CAPLUS Full-text
 DOCUMENT NUMBER: 135:92535
 TITLE: Process for the preparation of 3-(1-hydroxypentylidene)-5-nitro-3H-benzofuran-2-one and its ketone tautomeric form 3-(1-oxo-pentyl)-5-nitro-3H-benzofuran-2-one

INVENTOR(S): Schouteeten, Alain; Mordacq, Francoise
 PATENT ASSIGNEE(S): Clariant (France) S.A., Fr.
 SOURCE: Eur. Pat. Appl., 5 pp.

CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1116719	A2	20010718	EP 2001-810033	20010115
EP 1116719	A3	20011024		
EP 1116719	B1	20050406		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2803846	A1	20010720	FR 2000-523	20000117
FR 2803846	B1	20020405		
TW 564246	B	20031201	TW 2001-90100495	20010110
HU 2001000146	A2	20020128	HU 2001-146	20010115
AT 292630	T	20050415	AT 2001-810033	20010115
ES 2238408	T3	20050901	ES 2001-810033	20010115
NO 2001000265	A	20010718	NO 2001-265	20010116
JP 2001233870	A	20010828	JP 2001-7465	20010116
KR 788529	B1	20071224	KR 2001-2333	20010116
CN 1306000	A	20010801	CN 2001-101296	20010117
US 2001012900	A1	20010809	US 2001-761452	20010117
US 6515147	B2	20030204		
IN 2003MA00433	A	20070330	IN 2003-MA433	20030528
US 39755	E1	20070731	US 2005-50627	20050203
PRIORITY APPLN. INFO.:			FR 2000-523	A 20000117
			US 2001-761452	E 20010117

OTHER SOURCE(S): CASREACT 135:92535

AB 3-(1-Hydroxypentylidene)-5-nitro-3H-benzofuran-2-one, and to its ketone tautomeric form 3-(1-oxo-pentyl)-5-nitro-3H-benzofuran-2-one, are prepared in

high yield and selectivity by the reaction of 5-nitro-3H-benzofuran-2- one at >30° with pentanoic anhydride and a salt of pentanoic acid, optionally in the presence of pentanoic acid, then the resulting reaction mixture is acidified (e.g., sulfuric acid) and the precipitated product (m.p. 164°, DSC) collected by filtration.

L35 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 143:97254 CASREACT Full-text

TITLE: Process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of carboxybenzofuran derivatives, Friedel-Crafts acylation with alkoxybenzenes and dealkylation

INVENTOR(S): Schouteeten, Alain; Bleger, Francois; Mordacq, Francoise; Piron, Jerome

PATENT ASSIGNEE(S): Clariant France, Fr.

SOURCE: Fr. Demande, 22 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2864536	A1	20050701	FR 2003-15398	20031224
FR 2864536	B1	20060317		
WO 2005066149	A1	20050721	WO 2004-IB4158	20041215
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GR, ML, MR, NE, SN, TD, TG			
EP 1699772	A1	20060913	EP 2004-801395	20041215
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CN 1898226	A	20070117	CN 2004-80038285	20041215
JP 2007517012	T	20070628	JP 2006-546365	20041215
NO 2006002936	A	20060922	NO 2006-2936	20060623
IN 2006CN02324	A	20070706	IN 2006-CN2324	20060626
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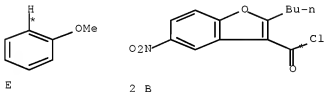
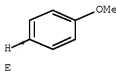
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

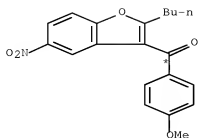
AB The invention is related to the preparation of benzofurans I [R = linear or branched alkyl; R1 = halo, NO₂, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C₆H₅OR₂ (III) [R₂ = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R₁, R₂ defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO₂; R₄ = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5-nitrobenzofuran with SOCl₂ in PhCl, acylation of anisole with acyl chloride in the presence of AlCl₃, and demethylation over AlCl₃ at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO₂, R = n-Bu] after purification. Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)-benzofuran in the presence of acetic anhydride/H₂SO₄ for 2 h gave acid II (m.p. = 207°).

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

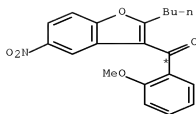
RX(2) OF 14 ...2 E + 2 B ==> F + G...



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F



G

RX(2)

STAGE(1)

RGT H 7446-70-0 AlCl₃

SOL 108-90-7 PhCl

CON room temperature -> 0 deg C

STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

STAGE(3)

RCT B 856758-03-7

CON SUBSTAGE(1) 1 hour, 5 deg C

SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C

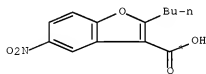
SUBSTAGE(3) 3 hours, room temperature

PRO F 141627-42-1, G 856758-04-8

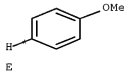
NTE Friedel-Crafts reaction, regioselective(4-methoxy product is the major isomer)

RX(6) OF 14 COMPOSED OF RX(1), RX(2)

RX(6) 2 A + 2 E ==> F + G



2 A



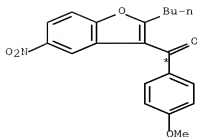
E



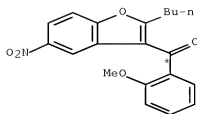
E

10/584440

2
STEPS
→



F



G

RX(1) RCT A 856758-02-6

STAGE(1)

SOL 108-90-7 PhCl

CON room temperature -> 80 deg C

STAGE(2)

RGT C 7719-09-7 SOC12

CON SUBSTAGE(1) 20 minutes, 80 deg C

SUBSTAGE(2) 9 hours, 80 deg C

PRO B 856758-03-7

NTE anisole alternately used as solvent

RX(2)

STAGE(1)

RGT H 7446-70-0 AlCl3

SOL 108-90-7 PhCl

CON room temperature -> 0 deg C

STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

STAGE(3)

RCT B 856758-03-7

CON SUBSTAGE(1) 1 hour, 5 deg C

SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C

SUBSTAGE(3) 3 hours, room temperature

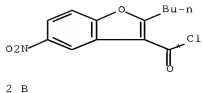
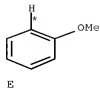
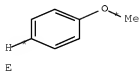
PRO F 141627-42-1, G 856758-04-8

NTE Friedel-Crafts reaction, regioselective(4-methoxy product is the major isomer)

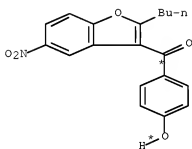
RX(7) OF 14 COMPOSED OF RX(2), RX(3)

RX(7) 2 E + 2 B ==> I

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2
STEPS
→



I

RX(2)

STAGE(1)

RGT H 7446-70-0 AlCl₃

SOL 108-90-7 PhCl

CON room temperature -> 0 deg C

STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

STAGE(3)

RCT B 856758-03-7

CON SUBSTAGE(1) 1 hour, 5 deg C

SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C

SUBSTAGE(3) 3 hours, room temperature

PRO F 141627-42-1, G 856758-04-8

NTE Friedel-Crafts reaction, regioselective(4-methoxy product is the major isomer)

RX(3)

RCT F 141627-42-1

STAGE(1)

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RGT H 7446-70-0 AlCl3
 SOL 108-90-7 PhCl
 CON 7 hours, room temperature -> 60 deg C

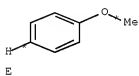
STAGE(2)

RGT J 7732-18-5 Water

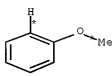
PRO I 141645-16-1

RX(8) OF 14 COMPOSED OF RX(2), RX(5)

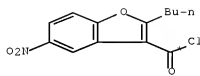
RX(8) 2 E + 2 E ==> I + N



E

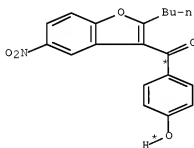


E

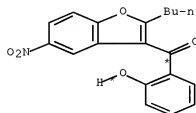


2 B

2
 STEPS
 →



I



N

RX(2)

STAGE(1)

RGT H 7446-70-0 AlCl3
 SOL 108-90-7 PhCl
 CON room temperature -> 0 deg C

STAGE(2)

RGT E 100-66-3
 CON 15 minutes, 0 deg C

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STAGE(3)

RCT B 856758-03-7

CON SUBSTAGE(1) 1 hour, 5 deg C

SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C

SUBSTAGE(3) 3 hours, room temperature

PRO F 141627-42-1, G 856758-04-8

NTE Friedel-Crafts reaction, regioselective(4-methoxy product is the major isomer)

RX(5) RCT F 141627-42-1, G 856758-04-8

STAGE(1)

RGT H 7446-70-0 AlCl3

SOL 108-90-7 PhCl

CON 7 hours, room temperature -> 60 deg C

STAGE(2)

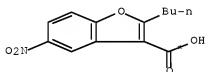
RGT J 7732-18-5 Water

CON 60 deg C

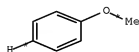
PRO I 141645-16-1, N 856758-05-9

RX(10) OF 14 COMPOSED OF RX(1), RX(2), RX(3)

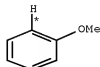
RX(10) 2 A + 2 E ==> I



2 A

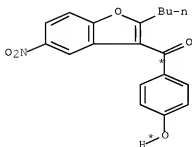


E



E

3
STEPS
→



I

10/584440

```
RX(1)      RCT  A 856758-02-6

            STAGE(1)
              SOL  108-90-7 PhCl
              CON  room temperature -> 80 deg C

            STAGE(2)
              RGT  C 7719-09-7 SOCl2
              CON  SUBSTAGE(1) 20 minutes, 80 deg C
                   SUBSTAGE(2) 9 hours, 80 deg C

PRO  B 856758-03-7
NTE  anisole alternately used as solvent

RX(2)

            STAGE(1)
              RGT  H 7446-70-0 AlCl3
              SOL  108-90-7 PhCl
              CON  room temperature -> 0 deg C

            STAGE(2)
              RCT  E 100-66-3
              CON  15 minutes, 0 deg C

            STAGE(3)
              RCT  B 856758-03-7
              CON  SUBSTAGE(1) 1 hour, 5 deg C
                   SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C
                   SUBSTAGE(3) 3 hours, room temperature

PRO  F 141627-42-1, G 856758-04-8
NTE  Friedel-Crafts reaction, regioselective(4-methoxy product is the
      major isomer)

RX(3)      RCT  F 141627-42-1

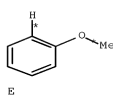
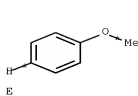
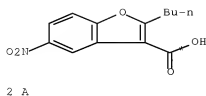
            STAGE(1)
              RGT  H 7446-70-0 AlCl3
              SOL  108-90-7 PhCl
              CON  7 hours, room temperature -> 60 deg C

            STAGE(2)
              RGT  J 7732-18-5 Water

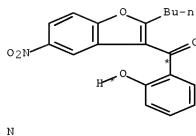
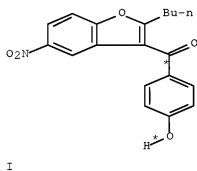
PRO  I 141645-16-1

RX(11) OF 14 COMPOSED OF RX(1), RX(2), RX(5)
RX(11)    2 A + 2 E ==> I + N
```

10/584440



3
STEPS
→



RX(1) RCT A 856756-02-6

STAGE(1)

SOL 108-90-7 PhCl

CON room temperature -> 80 deg C

STAGE(2)

RGT C 7719-09-7 SOCl2

CON SUBSTAGE(1) 20 minutes, 80 deg C

SUBSTAGE(2) 9 hours, 80 deg C

PRO B 856758-03-7

NTE anisole alternately used as solvent

RX(2)

STAGE(1)

RGT H 7446-70-0 AlCl3

SOL 108-90-7 PhCl

CON room temperature -> 0 deg C

STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

10/584440

```

      STAGE(3)
      RCT  B 856758-03-7
      CON  SUBSTAGE(1) 1 hour, 5 deg C
           SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C
           SUBSTAGE(3) 3 hours, room temperature

PRO  F 141627-42-1, G 856758-04-8
NTE  Friedel-Crafts reaction, regioselective(4-methoxy product is the
      major isomer)

RX(5)  RCT  F 141627-42-1, G 856758-04-8

      STAGE(1)
      RGT  H 7446-70-0 AlCl3
      SOL  108-90-7 PhCl
      CON  7 hours, room temperature -> 60 deg C

      STAGE(2)
      RGT  J 7732-18-5 Water
      CON  60 deg C

PRO  I 141645-16-1, N 856758-05-9
AN   143:97254  CASREACT  Full-text
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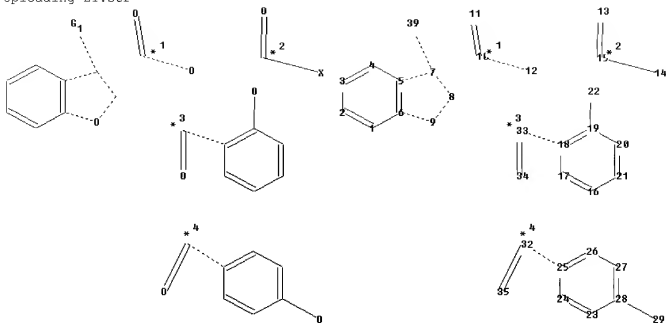
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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10/584440

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ring bonds :
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20-21 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
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exact bonds :
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normalized bonds :
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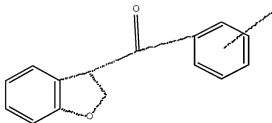
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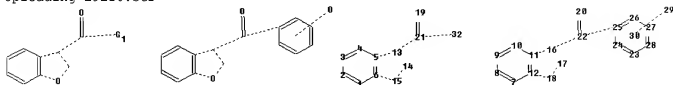
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L9 STR



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28
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ring bonds :
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21-32 22-25
normalized bonds :
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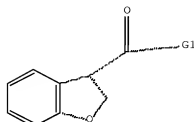
Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
32:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
node mappings:
14:17 13:16
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10/584440

L10

STR



G1 O,X

Structure attributes must be viewed using STN Express query preparation.

L12 1802 SEA FILE=REGISTRY SUB=L5 SSS FUL L9
L14 7056 SEA FILE=REGISTRY SUB=L5 SSS FUL L10
L17 230 SEA FILE=CAPLUS ABB=ON PLU=ON L12 (L) PREP/RL
L18 312 SEA FILE=CAPLUS ABB=ON PLU=ON L14 (L) (RACT OR RGT OR
RCT)/RL
L19 5 SEA FILE=CAPLUS ABB=ON PLU=ON L17 AND L18

=> s L19 not L36

L37 4 L19 NOT L36

=> file casreact

FILE 'CASREACT' ENTERED AT 10:47:51 ON 19 FEB 2008
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FILE CONTENT:1840 - 16 Feb 2008 VOL 148 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 13.8 million reactions   *
*
*****
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

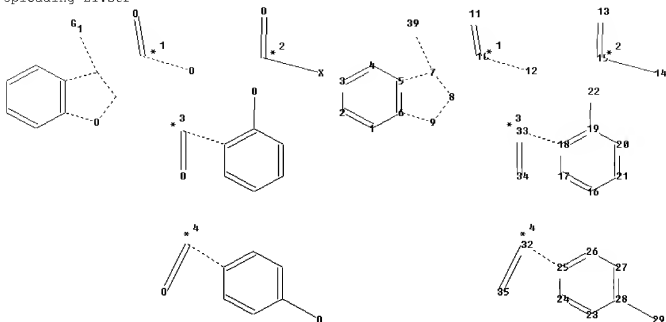
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L8

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
 Uploading L1.str



```

chain nodes :
10 11 12 13 14 15 22 29 32 33 34 35 39
ring nodes :
1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 28
chain bonds :
7-39 10-12 10-11 13-15 14-15 18-33 19-22 25-32 28-29 32-35 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 16-17 16-21 17-18 18-19 19-20
20-21 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-35
33-34
exact bonds :
14-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 23-24 23-
28
24-25 25-26 26-27 27-28

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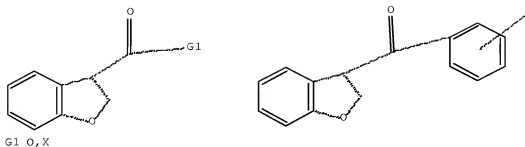
G1:[*1],[*2],[*3],[*4]

Match level :

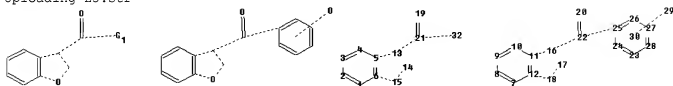
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS
33:CLASS
34:CLASS 35:CLASS 39:CLASS

```



Structure attributes must be viewed using SIN Express query preparation:
Uploading L3.str



```

chain nodes :
19 20 21 22 29 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27
28
chain bonds :
13-21 16-22 19-21 20-22 21-32 22-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-13 6-15 7-8 7-12 8-9 9-10 10-11 11-12 11-16
12-18 13-14 14-15 16-17 17-18 23-24 23-28 24-25 25-26 26-27 27-28
exact/norm bonds :
5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-22
21-32 22-25
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 23-24 23-28 24-
25
25-26 26-27 27-28

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G1:O,X

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
32:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
node mappings:
14:17 13:16

```

10/584440

L5 8858 SEA FILE=REGISTRY SSS FUL L1
L6 324 SEA FILE=CASREACT ABB=ON PLU=ON L5
L8 2 SEA FILE=CASREACT SUB=L6 SSS FUL L3 (8 REACTIONS)

100.0% DONE 254 VERIFIED 8 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.01

=> s l8 not L35
L38 1 L8 NOT L35

=> dup rem L38 L37
FILE 'CASREACT' ENTERED AT 10:48:16 ON 19 FEB 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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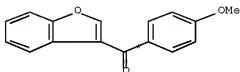
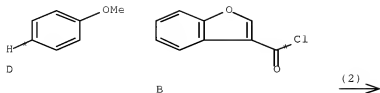
FILE 'CAPLUS' ENTERED AT 10:48:16 ON 19 FEB 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L37
L39 5 DUP REM L38 L37 (0 DUPLICATES REMOVED)
ANSWER '1' FROM FILE CASREACT
ANSWERS '2-5' FROM FILE CAPLUS

=> d ibib abs hit L39 1; d ibib abs hitind hitstr L39 2-5

L39 ANSWER 1 OF 5 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 108:21130 CASREACT Full-text
TITLE: Conformational analysis of organic carbonyl compounds.
Part 5. p-Methoxybenzoyl derivatives of
benzo[b]furan, benzo[b]thiophene, and naphthalene
AUTHOR(S): Benassi, Rois; Folli, Ugo; Larossi, Dario; Schenetti,
Luisa; Taddei, Ferdinando
CORPORATE SOURCE: Dip. Chim., Univ. Modena, Modena, 41100, Italy
SOURCE: Journal of the Chemical Society, Perkin Transactions
2: Physical Organic Chemistry (1972-1999) (1987),
(3), 351-7
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The conformational anal. of 2- and 3-(p-methoxybenzoyl)benzo[b]furan and -
benzo[b]thiophene and 1- and 2-(p-methoxybenzoyl)naphthalene was performed by
the NMR lanthanide-induced shift method on ¹H and ¹³C chemical shifts with
Yb(fod)₃. In the 2-substituted benzo[b]furan a chelate structure having the
lanthanide atom bound to both carbonyl and furyl oxygens is formed, so the
results do not represent useful information for the conformational properties
of the mol. in solution For the 2-benzo[b]thiophene derivative the S,O-cis
(Z) conformation was found to be more abundant in the equilibrium mixture of
the two nearly planar conformers. In the corresponding 3-substituted
heterocycles the predominant conformation is that of X,O-trans type with a
similar degree of distortion from planarity in the two compds. In all these
mols. the p-methoxyphenyl ring is twisted .apprx.30° from the carbonyl plane.

10/584440

RX(2) OF 4 ...D + B ==> E

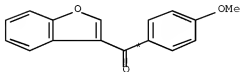
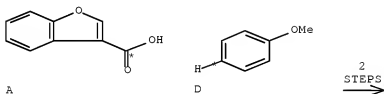


E
YIELD 44%

RX(2) RCT D 100-66-3, B 111964-21-7
 RGT F 7446-70-0 AlCl3
 PRO E 28222-80-2
 SOL 75-15-0 CS2

RX(4) OF 4 COMPOSED OF RX(1), RX(2)

RX(4) A + D ==> E



E
YIELD 44%

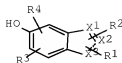
10/584440

RX(1) RCT A 26537-68-8
 RGT C 7719-09-7 SOC12
 PRO B 111964-21-7
 SOL 7719-09-7 SOC12

RX(2) RCT D 100-66-3, B 111964-21-7
 RGT F 7446-70-0 AIC13
 PRO E 28222-80-2
 SOL 75-15-0 CS2

L39 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:99174 CAPLUS Full-text
 DOCUMENT NUMBER: 142:198073
 TITLE: Preparation of heterocyclic compounds useful as
 malonyl-CoA decarboxylase inhibitors
 INVENTOR(S): Cheng, Jie Fei; Nguyen, Bao Ngoc; Liu, Xuwei;
 Lopaschuk, Gary D.; Dyck, Jason R.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 18 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005026969	A1	20050203	US 2004-900958	20040728
CA 2533747	A1	20050210	CA 2004-2533747	20040728
WO 2005011670	A1	20050210	WO 2004-US24285	20040728
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1653944	A1	20060510	EP 2004-757346	20040728
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007501232	T	20070125	JP 2006-522610	20040728
PRIORITY APPLN. INFO.: US 2003-492030P P 20030801 WO 2004-US24285 W 20040728				
OTHER SOURCE(S): CASREACT 142:198073; MARPAT 142:198073 GI				



I

- AB The present invention provides methods for the use of compds. I [X1, X2, X3 = O, N, NH, NR5, S, C; R1, R2 = H, halogen, substituted C1-6-alkyl, substituted C1-6-alkenyl, substituted C1-6-alkynyl, alkoxy, (un)substituted Ph, aryl, (un)substituted heteroaryl, NHCONR5R6, COR5, CONR5R6, S(O)nR5, SO2NR5R6; R3, R4 = H, Br, Cl, F, I, OH, OMe, CO2H, CO2R5, CONR5R6, S(O)nR5, SO2NR5R6, substituted C1-6-alkyl, C1-6-alkoxy, (un)substituted Ph, aryl, heteroaryl; R5, R6 = H, (un)substituted C1-6-alkyl, (un)substituted Ph, aryl, heteroaryl], its enantiomers, diastereomers, tautomers, or physiol. acceptable salts or prodrugs, pharmaceutical compns. containing the same, and methods for the prophylaxis, management and treatment of metabolic diseases and diseases modulated by MCD inhibition. Thus, benzofuran I [X1 = CC(:O)NHC6H3(OMe)2-3,4, X2 = CH, X3 = O, R3 = 4-Br, R4 = 6-Br] was prepared from 5-methoxybenzofuran-2-carboxylic acid via regioselective bromination at C(3), decarboxylation, debromination-carboxylation at C(3), O-demethylation, regioselective dibromination and amidation with 3,4-dimethoxyaniline. The compds. disclosed in this invention are useful for the prophylaxis, management and treatment of diseases involving in malonyl-CoA regulated glucose/fatty acid metabolism pathway. The inhibitory activity of I vs. malonyl-CoA decarboxylase was determined [Ki = 31.6 - 4750.2 μ M]. In particular, these compds. and pharmaceutical composition containing the same are indicated in the prophylaxis, management and treatment of cardiovascular diseases, diabetes, cancer and obesity.
- IC ICM A61K031-433
ICS A61K031-428; A61K031-4245; A61K031-423; A61K031-4184
- INCL 514363000; 514364000; 514367000; 514375000; 514394000
- CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7, 27, 63
- IT 23455-49-4E 383159-30-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-demethylation of; preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase inhibitors)
- IT 836629-05-1P, 4,6-Dibromo-5-hydroxybenzofuran-2-carboxylic acid 836629-06-2P, 4,6-Dibromo-5-hydroxybenzofuran-3-carboxylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of; preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase inhibitors)
- IT 29735-85-1P, 5-Hydroxybenzofuran-3-carboxylic acid 56172-36-2P, 5-Hydroxybenzofuran-2-carboxylic acid 251477-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of; preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase inhibitors)
- IT 41967-46-8P 41967-47-9P 412966-58-6P 836628-69-4P,

2-Benzoyl-4,6-dibromo-5-hydroxybenzofuran	836628-70-7P	836628-71-8P
836628-72-9P	836628-73-0P	836628-74-1P
836628-75-2P	836628-76-3P	836628-77-4P
836628-78-5P	836628-79-6P	836628-80-9P
836628-81-0P	836628-82-1P	836628-83-2P
836628-84-3P	836628-85-4P	836628-86-5P
836628-87-6P	836628-88-7P	836628-89-8P
836628-90-1P	836628-91-2P	836628-92-3P
836628-93-4P	836628-94-5P	836628-95-6P
836628-96-7P	836628-97-8P	836628-98-9P
836629-00-6P	836629-01-7P	836629-02-8P
836629-03-9P	836629-04-0P	836629-38-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);
USES (Uses)

(preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase inhibitors)

IT 23455-49-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

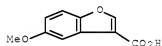
(preparation and O-demethylation of; preparation of heterocyclic compds.

useful

as malonyl-CoA decarboxylase inhibitors)

RN 23455-49-4 CAPLUS

CN 3-Benzofurancarboxylic acid, 5-methoxy- (CA INDEX NAME)



IT 836629-06-2P, 4,6-Dibromo-5-hydroxybenzofuran-3-carboxylic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

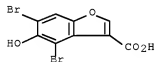
(preparation and amidation of; preparation of heterocyclic compds. useful

as

malonyl-CoA decarboxylase inhibitors)

RN 836629-06-2 CAPLUS

CN 3-Benzofurancarboxylic acid, 4,6-dibromo-5-hydroxy- (CA INDEX NAME)



IT 29735-85-1P, 5-Hydroxybenzofuran-3-carboxylic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

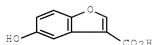
(preparation and bromination of; preparation of heterocyclic compds. useful

as

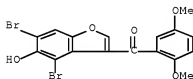
malonyl-CoA decarboxylase inhibitors)

RN 29735-85-1 CAPLUS

CN 3-Benzofurancarboxylic acid, 5-hydroxy- (CA INDEX NAME)



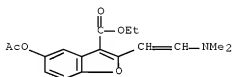
IT 412966-58-6P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase inhibitors)
 RN 412966-58-6 CAPLUS
 CN Methanone, (4,6-dibromo-5-hydroxy-3-benzofuranyl) (2,5-dimethoxyphenyl)- (CA INDEX NAME)



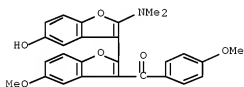
L39 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1997:8073 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 126:144080
 TITLE: β -(2-Benzofuranyl)enamines and (2-indolyl)enamines in the Nenitzescu reaction
 AUTHOR(S): Mukhanova, Tatyana I.; Panisheva, Elena K.; Lyubchanskaya, Valeriya M.; Alekseeva, Lyudmila M.; Sheinker, Yuriy N.; Granik, Vladimir G.
 CORPORATE SOURCE: Center for Drug Chemistry, All Russian Res. Chemical-Pharmaceutical Institute, Moscow, Russia
 SOURCE: Tetrahedron (1997), 53(1), 177-184
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Depending on the volume and electron-withdrawing properties of the substituents in the heterocyclic ring, reaction of β -(2-benzofuranyl)- and (2-indolyl)enamines with benzoquinone led to the formation of 3-heteroarylbenzofurans, with or without a dimethylamino group in the position 2. If dehydrogenation was impossible, as in the case of α -methyl- β -heteroarylenamines, furo[2,3-f]benzofurans are formed.
 CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 25
 IT 128944-24-1P 163890-14-0P 186553-66-2P 186553-75-3P
 186553-76-4P 186553-79-7P 186553-80-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)
 IT 186553-67-3P 186553-68-4P 186553-70-8P 186553-71-9P
 186553-72-0P 186553-73-1P 186553-74-2P 186553-77-5P
 186553-78-6P 186553-81-1P 186553-82-2P

10/584440

RL: SPN (Synthetic preparation); PREP (Preparation)
 (Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)
 IT 186553-66-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)
 RN 186553-66-2 CAPLUS
 CN 3-Benzofurancarboxylic acid, 5-(acetyloxy)-2-[2-(dimethylamino)ethenyl]-,
 ethyl ester (CA INDEX NAME)



IT 186553-72-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)
 RN 186553-72-0 CAPLUS
 CN Methanone, [2'-(dimethylamino)-5'-hydroxy-5-methoxy[2,3'-bibenzofuran]-3-yl][4-methoxyphenyl]- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1974:403757 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 81:3757
 ORIGINAL REFERENCE NO.: 81:607a,610a
 TITLE: Antiangina benzofuran derivatives
 INVENTOR(S): Descamps, Marcel; Gubin, Jean; Claeys, Norbert
 PATENT ASSIGNEE(S): Labaz
 SOURCE: Ger. Offen., 38 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2347196	A1	19740328	DE 1973-2347196	19730919
ZA 7305652	A	19741030	ZA 1973-5652	19730817

AU 7359650	A	19750227	AU 1973-59650	19730827
FI 55336	C	19790710	FI 1973-2715	19730831
FI 55336	B	19790330		
CA 983502	A1	19760210	CA 1973-180166	19730904
BE 804550	A1	19740306	BE 1973-135394	19730906
US 3920707	A	19751118	US 1973-395847	19730910
GB 1382742	A	19750205	GB 1972-43387	19730912
CH 579558	A5	19760915	CH 1973-13083	19730912
NL 7312817	A	19740321	NL 1973-12817	19730918
DK 133899	B	19760809	DK 1973-5094	19730918
SU 566523	A3	19770725	SU 1973-1962896	19730918
NO 138336	C	19780823	NO 1973-3641	19730918
JP 49069658	A	19740705	JP 1973-106477	19730919
AT 325034	B	19750925	AT 1973-8079	19730919
ES 418892	A1	19760301	ES 1973-418892	19730919
			GB 1972-43387	A 19720919

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

AB Benzofurans I (R = C1-4 alkyl, cyclohexyl; R1 = H, Me, Et, Pr; NR2R3 = NH2, alkylamino, dialkylamino, heterocyclic amino; n = 3-6) (70 compds.) were prepared. Thus I (R = Et, R1 = Me, NR2R3 = NBU2, n = 3) (II) was prepared by converting 2-ethyl-3-benzofurancarboxylic acid to its chloride, treating with 2,6-Me2C6H3OMe, ether cleavage of the 2-ethyl-3-(3,5-dimethyl-4-methoxybenzoyl)benzofuran, treating the hydroxy compound with Br(CH2)3Br and Bu2NH. II was as active as 2-butyl-3-(3,5-diiodo-4-(3,5-dimethylaminopropoxybenzoyl)benzofuran in reducing the heart rate of anesthetized dogs.

IC C07D; A61K

CC 27-7 (Heterocyclic Compounds (One Hetero Atom))

IT 52489-45-9P 52489-46-0P 52489-47-1P
 52489-48-2P 52489-49-3P 52489-50-6P
 52489-51-7P 52489-52-6P 52489-53-9P
 52489-54-0P 52489-55-1P 52489-56-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and ether cleavage of)

IT 52489-70-0P 52489-71-1P 52489-72-2P
 52489-73-3P 52489-74-4P 52490-16-1P
 52490-52-5P 52490-53-6P 52490-61-6P
 52490-62-7P 52490-69-4P 52490-70-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with amines)

IT 52489-35-7P 52489-36-8P 52489-37-9P
 52489-38-0P 52489-39-1P 52489-40-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with dialkylanisoles)

IT 52489-58-4P 52489-59-5P 52489-60-8P
 52489-61-9P 52489-62-0P 52489-63-1P
 52489-64-2P 52489-65-3P 52489-66-4P
 52489-67-5P 52489-68-6P 52489-69-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with dibromopropane)

IT 50602-48-7E 52489-75-5P 52489-76-6P
 52489-77-7E 52489-79-9P 52489-81-3E
 52489-83-5E 52489-85-7P 52489-87-9E
 52489-89-1P 52489-91-5P 52489-92-6P
 52489-93-7P 52489-94-8P 52489-95-9P
 52489-97-1P 52489-98-2P 52490-60-3P
 52490-61-4P 52490-63-6E 52490-65-8P

52490-06-9P 52490-07-0P 52490-08-1P
 52490-10-5P 52490-12-7P 52490-14-3P
 52490-17-2P 52490-19-4P 52490-21-8P
 52490-22-9P 52490-23-0P 52490-24-1P
 52490-25-2P 52490-27-4P 52490-28-5P
 52490-29-6P 52490-31-0P 52490-32-1P
 52490-33-2P 52490-35-4P 52490-36-5P
 52490-38-7P 52490-40-1P 52490-42-3P
 52490-44-5P 52490-46-7P 52490-48-9P
 52490-49-0P 52490-50-3P 52490-51-4P
 52490-55-8P 52490-56-9P 52490-58-1P
 52490-60-5P 52490-64-9P 52490-66-1P
 52490-68-3P 52490-72-9P 52490-74-1P
 52490-76-3P 52490-77-4P 52490-78-5P
 52490-79-6P 52490-80-9P 52490-81-0P
 52490-82-1P 52490-83-2P 52552-55-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT 3265-74-5 52489-34-6 52489-41-5

52489-42-6 52489-43-7 52489-44-8

RL: PCT (Reactant); PACT (Reactant or reagent)
 (reaction of, with thionyl chloride)

IT 52489-45-9P 52489-46-0P 52489-47-1P

52489-48-2P 52489-49-3P 52489-50-6P

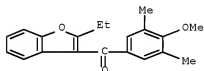
52489-51-7P 52489-52-8P 52489-53-9P

52489-54-0P 52489-55-1P 52489-56-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and ether cleavage of)

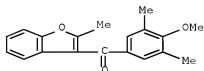
RN 52489-45-9 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) (4-methoxy-3,5-dimethylphenyl)- (CA
 INDEX NAME)



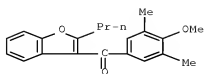
RN 52489-46-0 CAPLUS

CN Methanone, (4-methoxy-3,5-dimethylphenyl) (2-methyl-3-benzofuranyl)- (CA
 INDEX NAME)



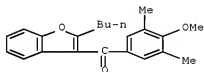
RN 52489-47-1 CAPLUS

CN Methanone, (4-methoxy-3,5-dimethylphenyl) (2-propyl-3-benzofuranyl)- (CA
 INDEX NAME)



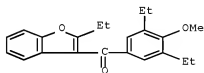
RN 52489-48-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) (4-methoxy-3,5-dimethylphenyl)- (CA INDEX NAME)



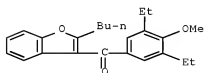
RN 52489-49-3 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl) (2-ethyl-3-benzofuranyl)- (CA INDEX NAME)



RN 52489-50-6 CAPLUS

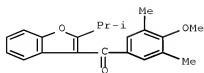
CN Methanone, (2-butyl-3-benzofuranyl) (3,5-diethyl-4-methoxyphenyl)- (CA INDEX NAME)



RN 52489-51-7 CAPLUS

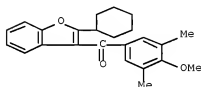
CN Methanone, (4-methoxy-3,5-dimethylphenyl) [2-(1-methylethyl)-3-benzofuranyl]- (CA INDEX NAME)

10/584440



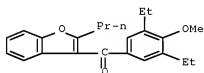
RN 52489-52-8 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl) (4-methoxy-3,5-dimethylphenyl)-
(CA INDEX NAME)



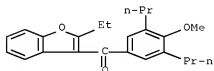
RN 52489-53-9 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl) (2-propyl-3-benzofuranyl)-
(CA INDEX NAME)



RN 52489-54-0 CAPLUS

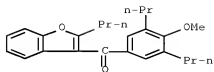
CN Methanone, (2-ethyl-3-benzofuranyl) (4-methoxy-3,5-dipropylphenyl)-
(CA INDEX NAME)



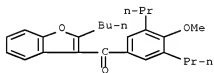
RN 52489-55-1 CAPLUS

CN Methanone, (4-methoxy-3,5-dipropylphenyl) (2-propyl-3-benzofuranyl)-
(CA INDEX NAME)

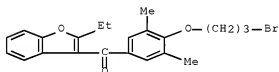
10/584440



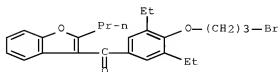
RN 52489-56-2 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl) (4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)



IT 52489-70-0P 52489-71-1P 52489-72-2P
52489-73-3P 52489-74-4P 52490-16-1P
52490-52-5P 52490-53-6P 52490-61-6P
52490-62-7P 52490-69-4P 52490-70-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(preparation); RACT (Reactant or reagent)
(preparation and reaction of, with amines)
RN 52489-70-0 CAPLUS
CN Methanone, [4-(3-bromopropoxy)-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-
(CA INDEX NAME)



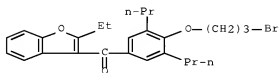
RN 52489-71-1 CAPLUS
CN Methanone, [4-(3-bromopropoxy)-3,5-diethylphenyl] (2-propyl-3-benzofuranyl)-
(CA INDEX NAME)



10/584440

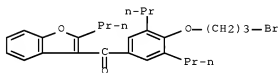
RN 52489-72-2 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-dipropylphenyl] (2-ethyl-3-benzofuranyl)-
(CA INDEX NAME)



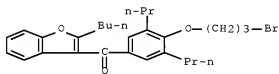
RN 52489-73-3 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-dipropylphenyl] (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



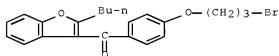
RN 52489-74-4 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-dipropylphenyl] (2-butyl-3-benzofuranyl)-
(CA INDEX NAME)



RN 52490-16-1 CAPLUS

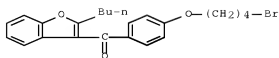
CN Methanone, [4-(3-bromopropoxy)phenyl] (2-butyl-3-benzofuranyl)- (CA INDEX NAME)



RN 52490-52-5 CAPLUS

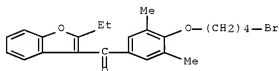
CN Methanone, [4-(4-bromobutoxy)phenyl] (2-butyl-3-benzofuranyl)- (CA INDEX NAME)

10/584440



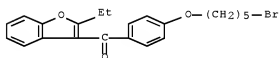
RN 52490-53-6 CAPLUS

CN Methanone, [4-(4-bromobutoxy)-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-
(CA INDEX NAME)



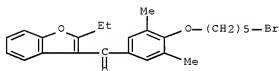
RN 52490-61-6 CAPLUS

CN Methanone, [4-[(5-bromopentyl)oxy]phenyl] (2-ethyl-3-benzofuranyl)- (CA
INDEX NAME)



RN 52490-62-7 CAPLUS

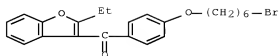
CN Methanone, [4-[(5-bromopentyl)oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)- (CA INDEX NAME)



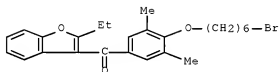
RN 52490-69-4 CAPLUS

CN Methanone, [4-[(6-bromohexyl)oxy]phenyl] (2-ethyl-3-benzofuranyl)- (CA
INDEX NAME)

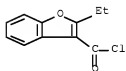
10/584440



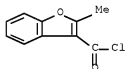
RN 52490-70-7 CAPLUS
 CN Methanone, [4-[(6-bromohexyl)oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)- (CA INDEX NAME)



IT 52489-35-7F 52489-36-8P 52489-37-9F
 52489-38-0F 52489-39-1P 52489-40-4F
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); PACT (Reactant or reagent)
 (preparation and reaction of, with dialkylanisoles)
 RN 52489-35-7 CAPLUS
 CN 3-Benzofurancarboxyl chloride, 2-ethyl- (CA INDEX NAME)

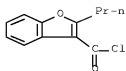


RN 52489-36-8 CAPLUS
 CN 3-Benzofurancarboxyl chloride, 2-methyl- (CA INDEX NAME)



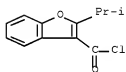
RN 52489-37-9 CAPLUS
 CN 3-Benzofurancarboxyl chloride, 2-propyl- (CA INDEX NAME)

10/584440



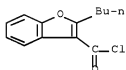
RN 52489-38-0 CAPLUS

CN 3-Benzofurancarboxyl chloride, 2-(1-methylethyl)- (CA INDEX NAME)



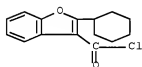
RN 52489-39-1 CAPLUS

CN 3-Benzofurancarboxyl chloride, 2-butyl- (CA INDEX NAME)



RN 52489-40-4 CAPLUS

CN 3-Benzofurancarboxyl chloride, 2-cyclohexyl- (CA INDEX NAME)



IT 52489-59-4F 52489-59-5P 52489-60-8F

52489-61-9F 52489-62-0P 52489-63-1F

52489-64-2F 52489-65-3P 52489-66-4F

52489-67-5P 52489-68-6P 52489-69-7P

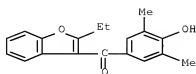
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with dibromopropane)

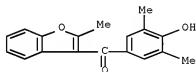
RN 52489-58-4 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)



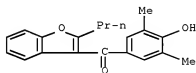
RN 52489-59-5 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl) (2-methyl-3-benzofuranyl)- (CA INDEX NAME)



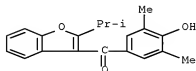
RN 52489-60-8 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl) (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



RN 52489-61-9 CAPLUS

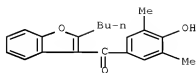
CN Methanone, (4-hydroxy-3,5-dimethylphenyl) [2-(1-methylethyl)-3-benzofuranyl]- (CA INDEX NAME)



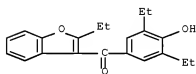
RN 52489-62-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

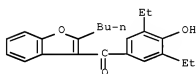
10/584440



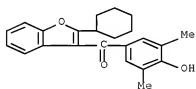
RN 52489-63-1 CAPLUS
CN Methanone, (3,5-diethyl-4-hydroxyphenyl) (2-ethyl-3-benzofuranyl)- (CA
INDEX NAME)



RN 52489-64-2 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl) (3,5-diethyl-4-hydroxyphenyl)- (CA
INDEX NAME)

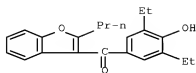


RN 52489-65-3 CAPLUS
CN Methanone, (2-cyclohexyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl)-
(CA INDEX NAME)

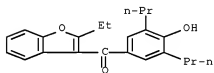


RN 52489-66-4 CAPLUS
CN Methanone, (3,5-diethyl-4-hydroxyphenyl) (2-propyl-3-benzofuranyl)- (CA
INDEX NAME)

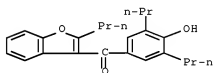
10/584440



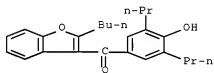
RN 52489-67-5 CAPLUS
CN Methanone, (2-ethyl-3-benzofuranyl) (4-hydroxy-3,5-dipropylphenyl)- (CA
INDEX NAME)



RN 52489-68-6 CAPLUS
CN Methanone, (4-hydroxy-3,5-dipropylphenyl) (2-propyl-3-benzofuranyl)- (CA
INDEX NAME)



RN 52489-69-7 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl) (4-hydroxy-3,5-dipropylphenyl)- (CA
INDEX NAME)



IT 50602-18-7P 52189-75-5P 52489-76-6P
52489-77-7P 52489-79-9P 52489-81-3P
52489-83-5P 52489-85-7P 52489-87-9P
52489-89-1P 52489-91-5P 52489-92-6P
52489-93-7P 52489-94-8P 52489-95-9P
52489-97-1P 52489-98-2P 52490-00-3P
52490-01-4P 52490-03-6P 52490-05-8P

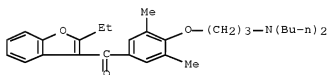
10/584440

52490-06-9P 52490-07-0P 52490-08-1P
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 52490-25-2P 52490-27-4P 52490-28-5P
 52490-29-6P 52490-31-0P 52490-32-1P
 52490-33-2P 52490-35-4P 52490-36-5P
 52490-38-7P 52490-40-1P 52490-42-3P
 52490-44-5P 52490-46-7P 52490-48-9P
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 52490-55-8P 52490-56-9P 52490-58-1P
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 52490-76-3P 52490-77-4P 52490-78-5P
 52490-79-6P 52490-80-9P 52490-81-0P
 52490-82-1P 52490-83-2P 52552-55-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 50602-48-7 CAPLUS

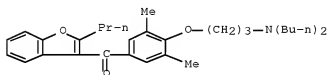
CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52489-75-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl] (2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

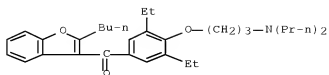


● HCl

RN 52489-76-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

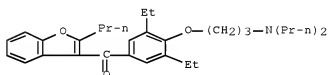
10/584440



● HCl

RN 52489-77-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl] (2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

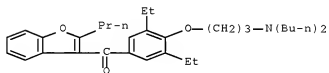
RN 52489-79-9 CAPLUS

CN Methanone, [4-[3-(diethylamino)propoxy]-3,5-diethylphenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-78-8

CMF C33 H47 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



10/584440

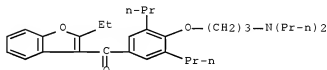
RN 52489-81-3 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-80-2

CMF C32 H45 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



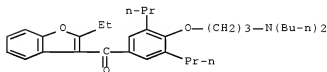
RN 52489-83-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-82-4

CMF C34 H49 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

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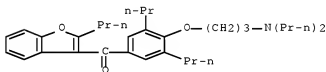
RN 52489-85-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-84-6

CMF C33 H47 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



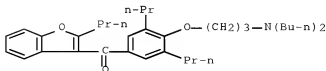
RN 52489-87-9 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-86-8

CMF C35 H51 N O3



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CM 2

CRN 144-62-7

CMF C2 H2 O4



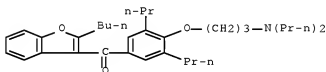
RN 52489-89-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-88-0

CMF C34 H49 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52489-91-5 CAPLUS

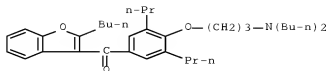
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-90-4

CMF C36 H53 N O3

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CM 2

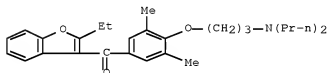
CRN 144-62-7

CMF C2 H2 O4



RN 52489-92-6 CAPLUS

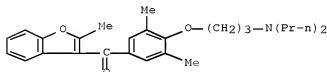
CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52489-93-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl] (2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



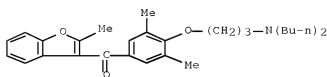
● HCl

RN 52489-94-8 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl] (2-methyl-3-

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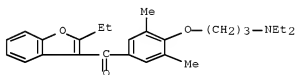
benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52489-95-9 CAPLUS

CN Methanone, [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

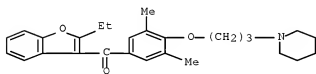
RN 52489-97-1 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(1-piperidinyl)propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-96-0

CMF C27 H33 N O3



CM 2

CRN 144-62-7

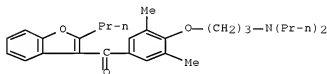
CMF C2 H2 O4

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RN 52489-98-2 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl] (2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



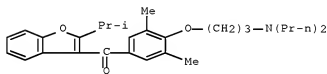
RN 52490-00-3 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl] [2-(1-methylethyl)-3-benzofuranyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-99-3

CMF C29 H39 N O3



CM 2

CRN 144-62-7

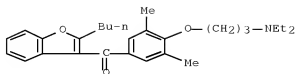
CMF C2 H2 O4



RN 52490-01-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

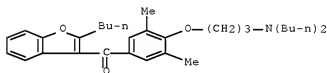
RN 52490-03-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-02-5

CMF C32 H45 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52490-05-8 CAPLUS

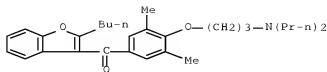
CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-04-7

CMF C30 H41 N O3

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CM 2

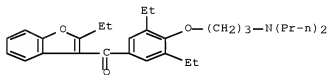
CRN 144-62-7

CMF C2 H2 O4



RN 52490-06-9 CAPLUS

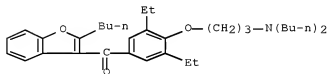
CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-07-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)



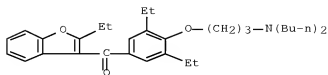
● HCl

RN 52490-08-1 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl] (2-ethyl-3-

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benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

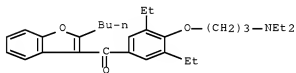
RN 52490-10-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]-3,5-diethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-09-2

CMF C30 H41 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52490-12-7 CAPLUS

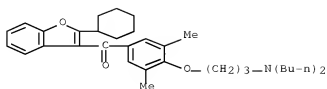
CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-11-6

CMF C34 H47 N O3

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CM 2

CRN 144-62-7

CMF C2 H2 O4



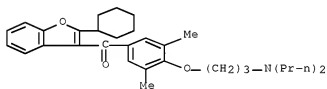
RN 52490-14-9 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-13-8

CMF C32 H43 N O3



CM 2

CRN 144-62-7

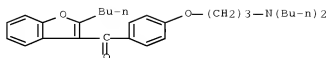
CMF C2 H2 O4



RN 52490-17-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

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● HCl

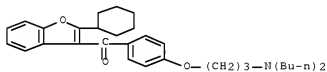
RN 52490-19-4 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-18-3

CMF C32 H43 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52490-21-8 CAPLUS

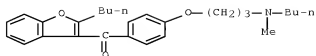
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylmethylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-20-7

CMF C27 H35 N O3

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CM 2

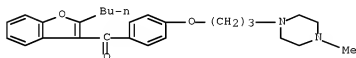
CRN 144-62-7

CMF C2 H2 O4



RN 52490-22-9 CAPLUS

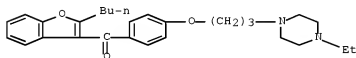
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-methyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 52490-23-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-ethyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

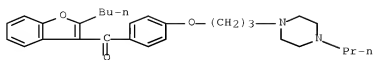


● 2 HCl

RN 52490-24-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-propyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

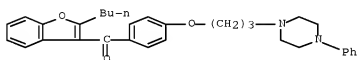
10/584440



● 2 HCl

RN 52490-25-2 CAPLUS

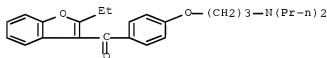
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-27-4 CAPLUS

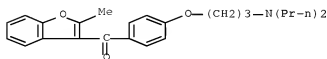
CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-28-5 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

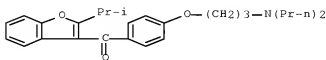


● HCl

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RN 52490-29-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

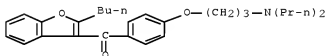
RN 52490-31-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-30-9

CMF C28 H37 N O3



CM 2

CRN 144-62-7

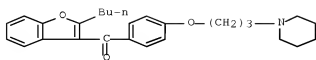
CMF C2 H2 O4



RN 52490-32-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(1-piperidinyl)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

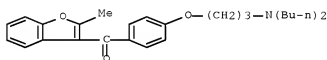
10/584440



● HCl

RN 52490-33-2 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl] (2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

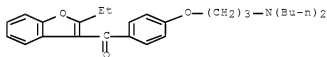
RN 52490-35-4 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-34-3

CMF C28 H37 N O3



CM 2

CRN 144-62-7

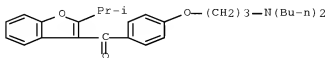
CMF C2 H2 O4



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RN 52490-36-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

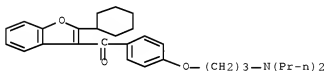
RN 52490-38-7 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-37-6

CMF C30 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52490-40-1 CAPLUS

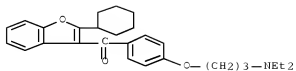
CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-39-8

CMF C28 H35 N O3

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CM 2

CRN 144-62-7

CMF C2 H2 O4



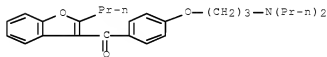
RN 52490-42-3 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-41-2

CMF C27 H35 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



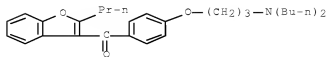
RN 52490-44-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

10/584440

CRN 52490-43-4
CMF C29 H39 N O3



CM 2

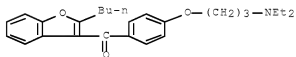
CRN 144-62-7
CMF C2 H2 O4



RN 52490-46-7 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-45-6
CMF C26 H33 N O3



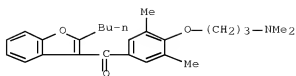
CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 52490-48-9 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dimethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

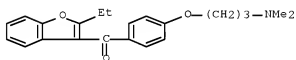
10/584440



● HCl

RN 52490-49-0 CAPLUS

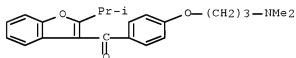
CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-50-3 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl] [2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

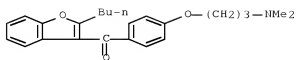


● HCl

RN 52490-51-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dimethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

10/584440

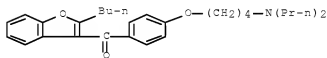


● HCl

RN 52490-55-8 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(dipropylamino)butoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-54-7
CMF C29 H39 N O3

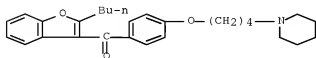


CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 52490-56-9 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(1-piperidinyl)butoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

10/584440

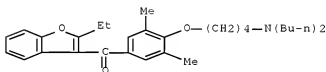
RN 52490-58-1 CAPLUS

CN Methanone, [4-[4-(dibutylamino)butoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-57-0

CMF C31 H43 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



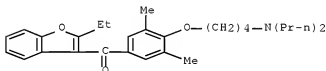
RN 52490-60-5 CAPLUS

CN Methanone, [4-[4-(dipropylamino)butoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-59-2

CMF C29 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

10/584440



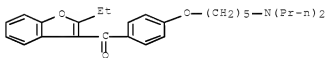
RN 52490-64-9 CAPLUS

CN Methanone, [4-[5-(dipropylamino)pentyl]oxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-63-8

CMF C28 H37 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



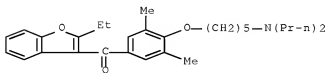
RN 52490-66-1 CAPLUS

CN Methanone, [4-[5-(dipropylamino)pentyl]oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-65-0

CMF C30 H41 N O3



CM 2

10/584440

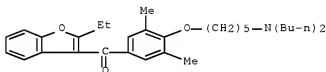
CRN 144-62-7
CMF C2 H2 O4



RN 52490-68-3 CAPLUS
CN Methanone, [4-[5-(dibutylamino)pentyl]oxy]-3,5-dimethylphenyl (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-67-2
CMF C32 H45 N O3



CM 2

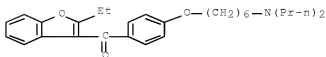
CRN 144-62-7
CMF C2 H2 O4



RN 52490-72-9 CAPLUS
CN Methanone, [4-[6-(dipropylamino)hexyl]oxy]phenyl (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-71-8
CMF C29 H39 N O3



10/584440

CM 2

CRN 144-62-7

CMF C2 H2 O4



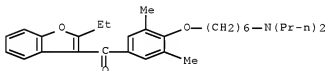
RN 52490-74-1 CAPLUS

CN Methanone, [4-[[6-(dipropylamino)hexyl]oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-73-0

CMF C31 H43 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52490-76-3 CAPLUS

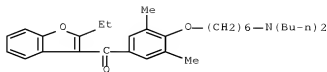
CN Methanone, [4-[[6-(dibutylamino)hexyl]oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-75-2

CMF C33 H47 N O3

10/584440



CM 2

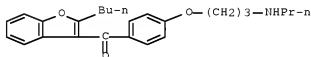
CRN 144-62-7

CMF C2 H2 O4



RN 52490-77-4 CAPLUS

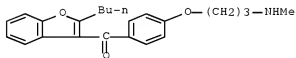
CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(propylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-78-5 CAPLUS

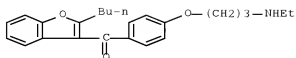
CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(methylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-79-6 CAPLUS

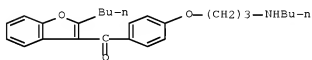
CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(ethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-80-9 CAPLUS

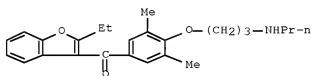
CN Methanone, [4-[3-(butylamino)propoxy]phenyl](2-butyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-81-0 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(propylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

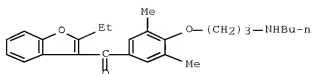


● HCl

RN 52490-82-1 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

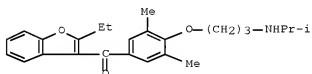
10/584440



● HCl

RN 52490-83-2 CAPLUS

CN Methanone, [3,5-dimethyl-4-{3-[(1-methylethyl)amino]propoxy}phenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

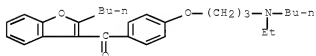
RN 52552-55-3 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-{3-(butylethylamino)propoxy}phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52552-54-2

CMF C28 H37 N O3



CM 2

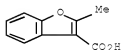
CRN 144-62-7

CMF C2 H2 O4

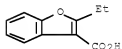


10/584440

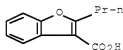
IT 3265-74-5 52489-34-6 52489-41-5
52489-42-6 52489-43-7 52489-44-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionyl chloride)
RN 3265-74-5 CAPLUS
CN 3-Benzofurancarboxylic acid, 2-methyl- (CA INDEX NAME)



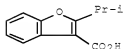
RN 52489-34-6 CAPLUS
CN 3-Benzofurancarboxylic acid, 2-ethyl- (CA INDEX NAME)



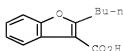
RN 52489-41-5 CAPLUS
CN 3-Benzofurancarboxylic acid, 2-propyl- (CA INDEX NAME)



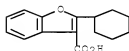
RN 52489-42-6 CAPLUS
CN 3-Benzofurancarboxylic acid, 2-(1-methylethyl)- (CA INDEX NAME)



RN 52489-43-7 CAPLUS
CN 3-Benzofurancarboxylic acid, 2-butyl- (CA INDEX NAME)



RN 52489-44-8 CAPLUS
 CN 3-Benzofurancarboxylic acid, 2-cyclohexyl- (CA INDEX NAME)



L39 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1974:437442 CAPLUS Full-text

DOCUMENT NUMBER: 81:37442

ORIGINAL REFERENCE NO.: 81:5995a,5998a

TITLE: Benzofuran series. LIV. Potential antianginal agents, 2-alkyl-3-(4-aminoalkoxy-3,5-dialkylbenzoyl)- and 3-(4-aminoalkoxybenzoyl)benzofurans

AUTHOR(S): Gubin, J.; Claeys, N.; Deray, E.; Descamps, M.; Bauthier, J.; Charlier, R.

CORPORATE SOURCE: Cent. Rech., S. A. Labaz N. V., Brussels, Belg.

SOURCE: European Journal of Medicinal Chemistry (1974), 9(1), 19-25

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE: Journal

LANGUAGE: French

GI For diagram(s), see printed CA Issue.

AB Benzofurans I (R = Me, Et, Pr, CHMe2, Bu, cyclohexyl; R1 = H, Me, Et, Pr, CHMe2; R2 = R3 = Me, Et, Pr, Bu; R1 = H, R1 = Me, Et, Pr, CHMe2, Bu; R2 = Bu, R3 = Me, Et; NR2R3 = piperidino, 4-Me[Et, Pr, Ph]-piperazino; n = 3-6) were prepared by alkylating II. II (R1 = Me, Et, Pr, CHMe2) were prepared by treating the (chlorocarbonyl)benzofuran with dialkylanisoles and cleaving the Me ether with pyridine-HCl. I are antianginal, although I (R1 = Pr, CHMe2) were inactive. Some, especially I (R = Et, R1 = Me, R2 = R3 = Bu, n = 3), were more active than amiodarone.

CC 27-7 (Heterocyclic Compounds (One Hetero Atom))

IT 52489-58-4P 52489-59-5P 52489-60-2P

52489-61-9P 52489-62-0P 52489-63-1P

52489-64-2P 52489-65-3P 52489-66-4P

52489-67-5P 52489-68-6P 52489-69-7P

52901-28-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and aminoalkylation of)

IT 52489-35-7P 52489-36-8P 52489-37-9P

52489-38-0P 52489-39-1P 52489-40-4P

RL: PCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and arylation of)

10/584440

IT 52489-45-5P 52489-46-0P 52489-47-1P
52489-48-2P 52489-49-3P 52489-50-6P
52489-52-8P 52489-53-9P 52489-54-0P
52489-55-1P 52489-56-2P 52901-64-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
{Preparation}; RACT (Reactant or reagent)

(preparation and demethylation of)

IT 3265-74-5P 50602-48-7P 52489-34-6P 52489-41-5P 52489-42-6P
52489-43-7P 52489-44-8P 52489-75-5P 52489-76-6P
52489-77-7P 52489-92-6P 52489-93-7P
52489-94-8P 52489-95-9P 52489-98-2P
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52490-56-9P 52490-77-4P 52490-78-5P
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52956-64-6P 52956-65-7P 52956-66-8P
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52956-70-4P 52956-71-5P 52949-34-6P

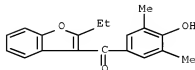
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 52489-58-4P 52489-59-5P 52489-60-8P
52489-61-9P 52489-62-0P 52489-63-1P
52489-64-2P 52489-65-3P 52489-66-4P
52489-67-5P 52489-68-6P 52489-69-7P
52901-28-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and aminoalkylation of)

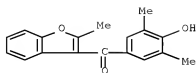
RN 52489-58-4 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl)- (CA
INDEX NAME)



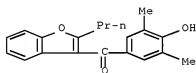
RN 52489-59-5 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl) (2-methyl-3-benzofuranyl)- (CA
INDEX NAME)



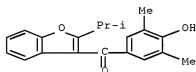
RN 52489-60-8 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl) (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



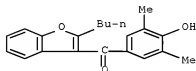
RN 52489-61-9 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl) [2-(1-methylethyl)-3-benzofuranyl]- (CA INDEX NAME)



RN 52489-62-0 CAPLUS

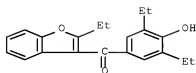
CN Methanone, (2-butyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)



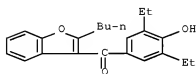
RN 52489-63-1 CAPLUS

CN Methanone, (3,5-diethyl-4-hydroxyphenyl) (2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

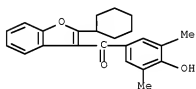
10/584440



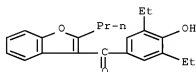
RN 52489-64-2 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl) (3,5-diethyl-4-hydroxyphenyl)- (CA INDEX NAME)



RN 52489-65-3 CAPLUS
CN Methanone, (2-cyclohexyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

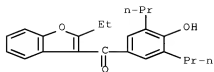


RN 52489-66-4 CAPLUS
CN Methanone, (3,5-diethyl-4-hydroxyphenyl) (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



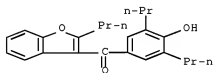
RN 52489-67-5 CAPLUS
CN Methanone, (2-ethyl-3-benzofuranyl) (4-hydroxy-3,5-dipropylphenyl)- (CA INDEX NAME)

10/584440



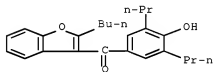
RN 52489-68-6 CAPLUS

CN Methanone, (4-hydroxy-3,5-dipropylphenyl) (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



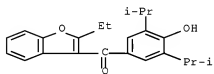
RN 52489-69-7 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) (4-hydroxy-3,5-dipropylphenyl)- (CA INDEX NAME)



RN 52901-28-7 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) [4-hydroxy-3,5-bis(1-methylethyl)phenyl]- (CA INDEX NAME)



IT 52489-35-7P 52189-36-8P 52489-37-9P

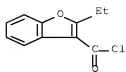
52489-38-6P 52489-39-1P 52489-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and arylation of)

RN 52489-35-7 CAPLUS

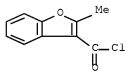
CN 3-Benzofurancarboxyl chloride, 2-ethyl- (CA INDEX NAME)

10/584440



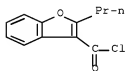
RN 52489-36-8 CAPLUS

CN 3-Benzofurancarboxyl chloride, 2-methyl- (CA INDEX NAME)



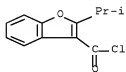
RN 52489-37-9 CAPLUS

CN 3-Benzofurancarboxyl chloride, 2-propyl- (CA INDEX NAME)



RN 52489-38-0 CAPLUS

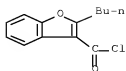
CN 3-Benzofurancarboxyl chloride, 2-(1-methylethyl)- (CA INDEX NAME)



RN 52489-39-1 CAPLUS

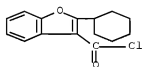
CN 3-Benzofurancarboxyl chloride, 2-butyl- (CA INDEX NAME)

10/584440



RN 52489-40-4 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-cyclohexyl- (CA INDEX NAME)



IT 52489-45-9P 52489-46-0P 52489-47-1P

52489-48-2P 52489-49-3P 52489-50-6P

52489-52-8P 52489-53-9P 52489-54-0P

52489-55-1P 52489-56-2P 52901-64-1P

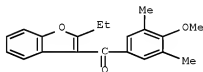
RL: RCT (Reactant); SPN (Synthetic preparation); PEP

(Preparation); RACT (Reactant or reagent)

(preparation and demethylation of)

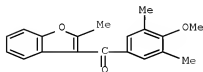
RN 52489-45-9 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) (4-methoxy-3,5-dimethylphenyl)- (CA INDEX NAME)



RN 52489-46-0 CAPLUS

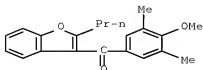
CN Methanone, (4-methoxy-3,5-dimethylphenyl) (2-methyl-3-benzofuranyl)- (CA INDEX NAME)



RN 52489-47-1 CAPLUS

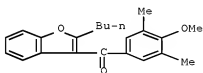
10/584440

CN Methanone, (4-methoxy-3,5-dimethylphenyl) (2-propyl-3-benzofuranyl)- (CA
INDEX NAME)



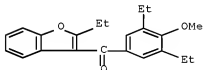
RN 52489-48-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) (4-methoxy-3,5-dimethylphenyl)- (CA
INDEX NAME)



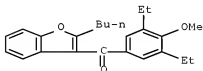
RN 52489-49-3 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl) (2-ethyl-3-benzofuranyl)- (CA
INDEX NAME)



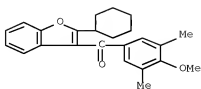
RN 52489-50-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) (3,5-diethyl-4-methoxyphenyl)- (CA
INDEX NAME)



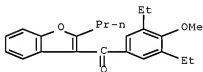
RN 52489-52-8 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl) (4-methoxy-3,5-dimethylphenyl)-
(CA INDEX NAME)



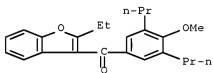
RN 52489-53-9 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl) (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



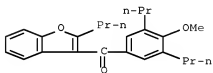
RN 52489-54-0 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) (4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)



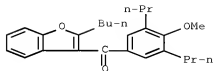
RN 52489-55-1 CAPLUS

CN Methanone, (4-methoxy-3,5-dipropylphenyl) (2-propyl-3-benzofuranyl)- (CA INDEX NAME)



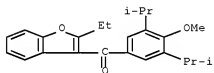
RN 52489-56-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) (4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)



RN 52901-64-1 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl) [4-methoxy-3,5-bis(1-methylethyl)phenyl]- (CA INDEX NAME)



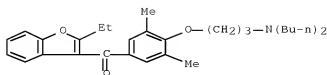
IT 50602-48-7P 52489-75-5P 52489-76-6P
 52489-77-7P 52489-92-6P 52489-93-7P
 52489-94-8P 52489-95-9P 52489-98-2P
 52490-01-4P 52490-06-9P 52490-07-0P
 52490-08-1P 52490-17-2P 52490-22-9P
 52490-23-0P 52490-24-1P 52490-25-2P
 52490-27-4P 52490-28-5P 52490-29-6P
 52490-32-1P 52490-33-2P 52490-36-5P
 52490-48-9P 52490-50-3P 52490-51-4P
 52490-56-9P 52490-77-4P 52490-78-5P
 52490-79-6P 52490-80-9P 52490-81-0P
 52490-82-1P 52490-83-2P 52901-30-1P
 52901-31-2P 52901-32-3P 52901-33-4P
 52901-34-5P 52901-35-6P 52901-36-7P
 52901-37-6P 52901-38-9P 52901-39-0P
 52901-40-3P 52901-41-4P 52901-42-5P
 52901-43-6P 52901-44-7P 52901-45-8P
 52901-46-9P 52901-48-1P 52901-49-2P
 52901-51-6P 52901-52-7P 52901-53-8P
 52901-54-9P 52901-55-0P 52901-56-1P
 52901-57-2P 52901-58-3P 52901-59-4P
 52956-64-6P 52956-65-7P 52956-66-8P
 52956-67-9P 52956-68-0P 52956-69-1P
 52956-70-4P 52956-71-5P 53049-34-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 50602-48-7 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

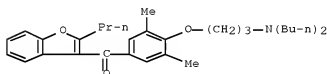
10/584440



● HCl

RN 52489-75-5 CAPLUS

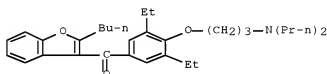
CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl] (2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52489-76-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

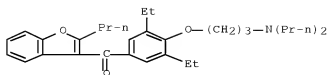


● HCl

RN 52489-77-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl] (2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

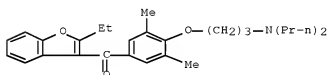
10/584440



● HCl

RN 52489-92-6 CAPLUS

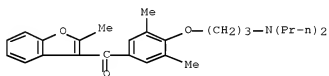
CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52489-93-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl] (2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

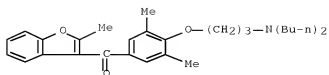


● HCl

RN 52489-94-8 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl] (2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

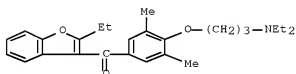
10/584440



● HCl

RN 52489-95-9 CAPLUS

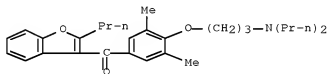
CN Methanone, [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52489-98-2 CAPLUS

CN Methanone, [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl] (2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

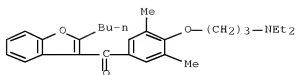


● HCl

RN 52490-01-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

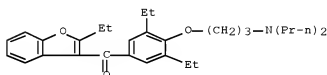
10/584440



● HCl

RN 52490-06-9 CAPLUS

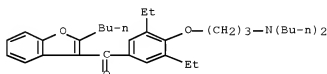
CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-07-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

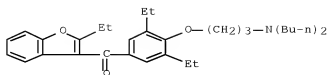


● HCl

RN 52490-08-1 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

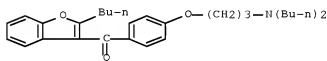
10/584440



● HCl

RN 52490-17-2 CAPLUS

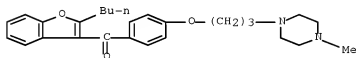
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-22-9 CAPLUS

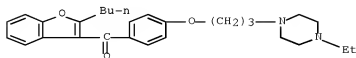
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-methyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 52490-23-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-ethyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

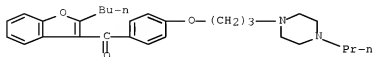


●2 HCl

10/584440

RN 52490-24-1 CAPLUS

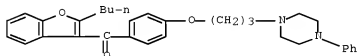
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-propyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 52490-25-2 CAPLUS

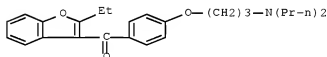
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-27-4 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

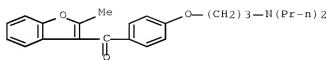


● HCl

RN 52490-28-5 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

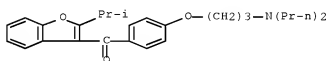
10/584440



● HCl

RN 52490-29-6 CAPLUS

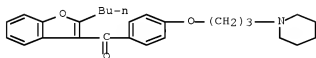
CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-32-1 CAPLUS

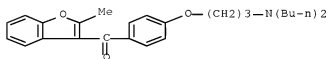
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(1-piperidinyl)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-33-2 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl][2-methyl-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

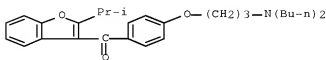


● HCl

10/584440

RN 52490-36-5 CAPLUS

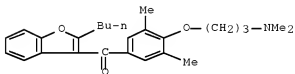
CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-48-9 CAPLUS

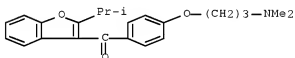
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dimethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-50-3 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

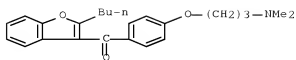


● HCl

RN 52490-51-4 CAPLUS

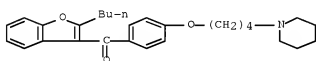
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dimethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

10/584440



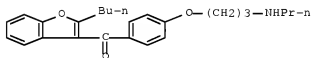
● HCl

RN 52490-56-9 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(1-piperidinyl)butoxy]phenyl]-,
hydrochloride (9CI) (CA INDEX NAME)



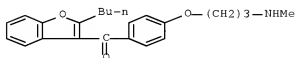
● HCl

RN 52490-77-4 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(propylamino)propoxy]phenyl]-,
hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-78-5 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(methylamino)propoxy]phenyl]-,
hydrochloride (9CI) (CA INDEX NAME)

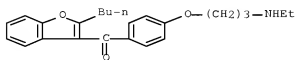


● HCl

10/584440

RN 52490-79-6 CAPLUS

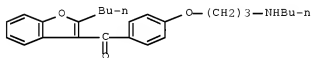
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(ethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-80-9 CAPLUS

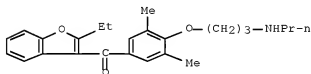
CN Methanone, [4-[3-(butylamino)propoxy]phenyl](2-butyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 52490-81-0 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(propylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

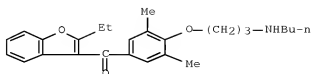


● HCl

RN 52490-82-1 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

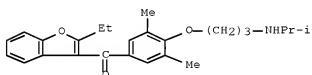
10/584440



● HCl

RN 52490-83-2 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-[(1-methylethyl)amino]propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

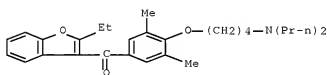
RN 52901-30-1 CAPLUS

CN Methanone, [4-[4-(dipropylamino)butoxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-59-2

CMF C29 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



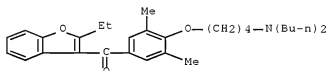
10/584440

RN 52901-31-2 CAPLUS
 CN Methanone, [4-[4-(dibutylamino)butoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-57-0

CMF C31 H43 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

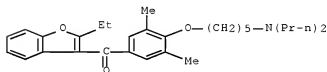


RN 52901-32-3 CAPLUS
 CN Methanone, [4-[5-(dipropylamino)pentyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-65-0

CMF C30 H41 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

10/584440



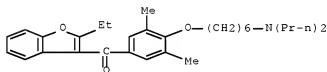
RN 52901-33-4 CAPLUS

CN Methanone, [4-[[6-(dipropylamino)hexyl]oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-73-0

CMF C31 H43 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



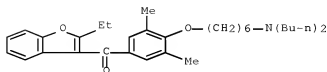
RN 52901-34-5 CAPLUS

CN Methanone, [4-[[6-(dibutylamino)hexyl]oxy]-3,5-dimethylphenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-75-2

CMF C33 H47 N O3



10/584440

CM 2

CRN 144-62-7

CMF C2 H2 O4



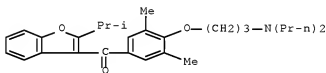
RN 52901-35-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl][2-(1-methylethyl)-3-benzofuranyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-99-3

CMF C29 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52901-36-7 CAPLUS

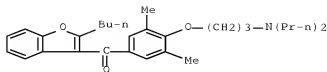
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-04-7

CMF C30 H41 N O3

10/584440



CM 2

CRN 144-62-7

CMF C2 H2 O4



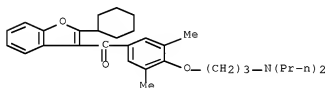
RN 52901-37-8 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-13-8

CMF C32 H43 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52901-38-9 CAPLUS

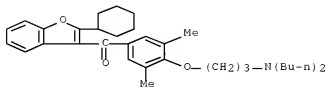
CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

10/584440

CM 1

CRN 52490-11-6

CMF C34 H47 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



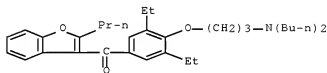
RN 52901-39-0 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-78-8

CMF C33 H47 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



10/584440

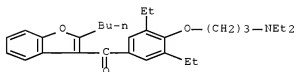
RN 52901-40-3 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]-3,5-diethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-09-2

CMF C30 H41 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



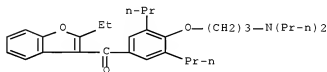
RN 52901-41-4 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-80-2

CMF C32 H45 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

10/584440



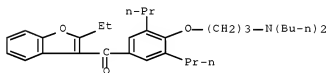
RN 52901-42-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-82-4

CMF C34 H49 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



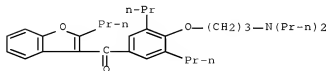
RN 52901-43-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-84-6

CMF C33 H47 N O3



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CM 2

CRN 144-62-7

CMF C2 H2 O4



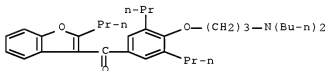
RN 52901-44-7 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-86-8

CMF C35 H51 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52901-45-8 CAPLUS

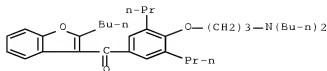
CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-90-4

CMF C36 H53 N O3

10/584440



CM 2

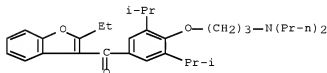
CRN 144-62-7

CMF C2 H2 O4



RN 52901-46-9 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-bis(1-methylethyl)phenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

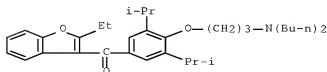
RN 52901-48-1 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-bis(1-methylethyl)phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52901-47-0

CMF C34 H49 N O3



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CM 2

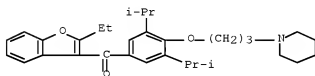
CRN 144-62-7

CMF C2 H2 O4



RN 52901-49-2 CAPLUS

CN Methanone, [3,5-bis(1-methylethyl)-4-[3-(1-piperidiny)propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

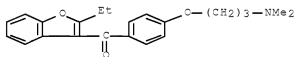
RN 52901-51-6 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52901-50-5

CMF C22 H25 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



10/584440

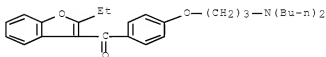
RN 52901-52-7 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-34-3

CMF C28 H37 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



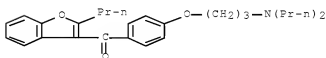
RN 52901-53-8 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-41-2

CMF C27 H35 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

10/584440



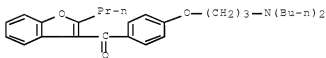
RN 52901-54-9 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl] (2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-43-4

CMF C29 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



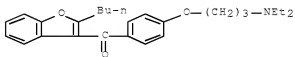
RN 52901-55-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-45-6

CMF C26 H33 N O3



CM 2

CRN 144-62-7

10/584440

CMF C2 H2 O4



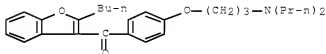
RN 52901-56-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-30-9

CMF C28 H37 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



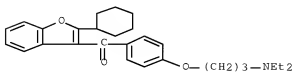
RN 52901-57-2 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-39-8

CMF C28 H35 N O3



10/584440

CM 2

CRN 144-62-7

CMF C2 H2 O4



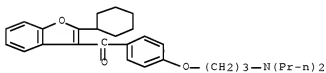
RN 52901-58-3 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-37-6

CMF C30 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 52901-59-4 CAPLUS

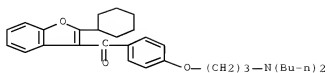
CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-18-3

CMF C32 H43 N O3

10/584440



CM 2

CRN 144-62-7

CMF C2 H2 O4



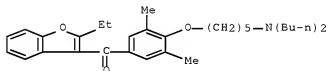
RN 52956-64-6 CAPLUS

CN Methanone, [4-[[5-(dibutylamino)pentyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-67-2

CMF C32 H45 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



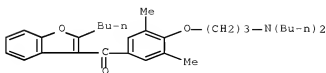
RN 52956-65-7 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

10/584440

CRN 52490-02-5
CMF C32 H45 N O3



CM 2

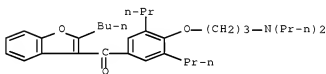
CRN 144-62-7
CMF C2 H2 O4



RN 52956-66-8 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-88-0
CMF C34 H49 N O3



CM 2

CRN 144-62-7
CMF C2 H2 O4



10/584440

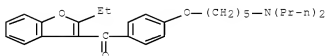
RN 52956-67-9 CAPLUS

CN Methanone, [4-[15-(dipropylamino)pentyl]oxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-63-8

CMF C28 H37 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



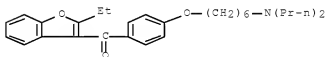
RN 52956-68-0 CAPLUS

CN Methanone, [4-[16-(dipropylamino)hexyl]oxy]phenyl] (2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-71-8

CMF C29 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



10/584440

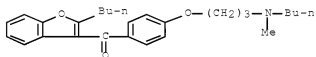
RN 52956-69-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylmethylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-20-7

CMF C27 H35 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



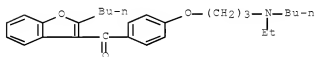
RN 52956-70-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylethylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52552-54-2

CMF C28 H37 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4

10/584440



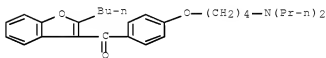
RN 52956-71-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(dipropylamino)butoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-54-7

CMF C29 H39 N O3



CM 2

CRN 144-62-7

CMF C2 H2 O4



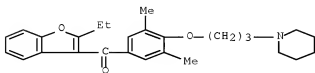
RN 53049-34-6 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(1-piperidiny)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-96-0

CMF C27 H33 N O3



CM 2

10/584440

CRN 144-62-7
CME C2 H2 O4



=> d his full

(FILE 'HOME' ENTERED AT 10:28:42 ON 19 FEB 2008)

FILE 'REGISTRY' ENTERED AT 10:28:53 ON 19 FEB 2008

L1 STRUCTURE UPLOADED
 L2 50 SEA SSS SAM L1

FILE 'STNGUIDE' ENTERED AT 10:30:21 ON 19 FEB 2008

L3 FILE 'CASREACT' ENTERED AT 10:33:31 ON 19 FEB 2008
 L4 STRUCTURE UPLOADED
 0 SEA SSS SAM L3 (0 REACTIONS)

FILE 'REGISTRY' ENTERED AT 10:35:51 ON 19 FEB 2008

L5 D STAT QUE L2
 8858 SEA SSS FUL L1
 SAVE TEMP L5 CHA440STR1L/A

FILE 'CASREACT' ENTERED AT 10:36:26 ON 19 FEB 2008

L6 324 SEA ABB=ON PLU=ON L5
 L7 0 SEA SUB=L6 SSS SAM L3 (0 REACTIONS)
 L8 2 SEA SUB=L6 SSS FUL L3 (8 REACTIONS)
 D SCA

FILE 'REGISTRY' ENTERED AT 10:37:52 ON 19 FEB 2008

L9 STRUCTURE UPLOADED
 L10 STRUCTURE UPLOADED
 L11 50 SEA SUB=L5 SSS SAM L9
 L12 1802 SEA SUB=L5 SSS FUL L9
 L13 50 SEA SUB=L5 SSS SAM L10
 L14 7056 SEA SUB=L5 SSS FUL L10
 L15 0 SEA ABB=ON PLU=ON L12 AND L13
 L16 0 SEA ABB=ON PLU=ON L12 AND L14

FILE 'CAPLUS' ENTERED AT 10:40:32 ON 19 FEB 2008

L17 230 SEA ABB=ON PLU=ON L12 (L) PREP/RL
 L18 312 SEA ABB=ON PLU=ON L14 (L) (RACT OR RGT OR RCT)/RL
 L19 5 SEA ABB=ON PLU=ON L17 AND L18
 L20 0 SEA ABB=ON PLU=ON SHOUTTEETEN A?/AU
 L21 4 SEA ABB=ON PLU=ON BLEGER F?/AU
 L22 2 SEA ABB=ON PLU=ON MORDACQ F?/AU
 L23 66 SEA ABB=ON PLU=ON PIRON J?/AU
 L24 1 SEA ABB=ON PLU=ON L21 AND L22 AND L23
 D AU
 L25 0 SEA ABB=ON PLU=ON SCHOUTEETAN A?/AU
 L26 37 SEA ABB=ON PLU=ON SCHOUTEETEN A?/AU
 L27 2 SEA ABB=ON PLU=ON L21 AND (L22 OR L23 OR L26)
 L28 2 SEA ABB=ON PLU=ON L22 AND (L23 OR L26)
 L29 1 SEA ABB=ON PLU=ON L23 AND L26
 L30 3 SEA ABB=ON PLU=ON (L27 OR L28 OR L29)
 L31 1 SEA ABB=ON PLU=ON L19 AND (L21 OR L22 OR L23 OR L26)
 L32 2 SEA ABB=ON PLU=ON L8
 L33 1 SEA ABB=ON PLU=ON L32 AND (L21 OR L22 OR L23 OR L26)
 SEL AN

FILE 'CASREACT' ENTERED AT 10:44:31 ON 19 FEB 2008

L34 1 SEA ABB=ON PLU=ON ("143:97254"/AN OR "2005:569050"/AN)

10/584440

L35 1 SEA ABB=ON PLU=ON L34 AND L8

FILE 'REGISTRY' ENTERED AT 10:45:40 ON 19 FEB 2008

FILE 'CAPLUS' ENTERED AT 10:45:42 ON 19 FEB 2008
D STAT QUE L30
D STAT QUE L31

L36 3 SEA ABB=ON PLU=ON L30 OR L31

FILE 'CASREACT' ENTERED AT 10:46:02 ON 19 FEB 2008
D STAT QUE L35

FILE 'CAPLUS' ENTERED AT 10:46:58 ON 19 FEB 2008
D IBIB ABS HITSTR L36 1-3

FILE 'CASREACT' ENTERED AT 10:46:59 ON 19 FEB 2008
D IBIB ABS HIT L35 1

FILE 'REGISTRY' ENTERED AT 10:47:22 ON 19 FEB 2008

FILE 'CAPLUS' ENTERED AT 10:47:24 ON 19 FEB 2008
D STAT QUE L19

L37 4 SEA ABB=ON PLU=ON L19 NOT L36

FILE 'CASREACT' ENTERED AT 10:47:51 ON 19 FEB 2008
D STAT QUE L8

L38 1 SEA ABB=ON PLU=ON L8 NOT L35

FILE 'CASREACT, CAPLUS' ENTERED AT 10:48:16 ON 19 FEB 2008

L39 5 DUP REM L38 L37 (0 DUPLICATES REMOVED)
ANSWER '1' FROM FILE CASREACT
ANSWERS '2-5' FROM FILE CAPLUS
D IBIB ABS HIT L39 1
D IBIB ABS HITIND HITSTR L39 2-5

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7
DICTIONARY FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE STNGUIDE

10/584440

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 15, 2008 (20080215/UP).

FILE CASREACT

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FILE CONTENT:1840 - 16 Feb 2008 VOL 148 ISS 8

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*          CASREACT now has more than 13.8 million reactions          *
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CAPLUS

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FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

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<http://www.cas.org/infopolicy.html>

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